

# The relationship between minimum gap and success probability in adiabatic quantum computing

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## Abstract

We explore the relationship between two figures of merit for an adiabatic quantum computation process: the success probability and the minimum gap between the ground and first excited states. We study a generic adiabatic algorithm and show that a rich structure exists in the distribution of these two important variables. In the case of two qubits, the success probability is to a good approximation a function of the minimum gap, the stage in the evolution at which the minimum occurs and the computation time. This structure persists in examples of larger systems and appears to be closely linked to the choice of initial and problem Hamiltonians.

## 1 Introduction

The promise of a qualitative advantage of quantum computers over classical ones in solving certain classes of problems has led to a massive effort in theoretical and experimental investigation of controlled, quantum-coherent systems. The standard model of quantum computing is analogous to classical computing in that it involves the precise manipulation of individual qubits in a register to apply logic gate operations. However, the requirement of precise time-dependent control of individual qubits has been found to be hard to achieve experimentally while still maintaining the quantum coherence of the system. A number of alternative approaches have been proposed, of which *adiabatic quantum computing* (AQC) is a promising example. It involves the evolution of a quantum system from a simple Hamiltonian with an easily-prepared ground state to a Hamiltonian that encodes the problem to be solved. If the system is initially

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prepared in the ground state and the time evolution occurs slowly enough to satisfy the adiabatic theorem, the final ground state that satisfies the problem at hand can be read out with a high probability [1].

The AQC process requires a Hamiltonian that interpolates from a simple initial configuration,  $H_i$ , to one that encodes the problem under consideration,  $H_f$ . A Hamiltonian for linear interpolation can be written

$$H(s) = (1 - s)H_i + sH_f, \quad (1)$$

where  $s \in [0, 1]$  is the reduced time  $s = t/T$ ,  $T$  being the computation time. The instantaneous eigenvalues and eigenstates of the Hamiltonian of an  $n$ -qubit system are given by

$$H(s) |\ell; s\rangle = E_\ell(s) |\ell; s\rangle, \text{ with } E_0(s) \leq E_1(s) \leq \dots \leq E_{2^n-1}(s). \quad (2)$$

The instantaneous state of the system is given by  $|\psi(s)\rangle$ , the solution of Schrödinger's equation, which in the reduced time reads

$$\frac{d}{ds} |\psi(s)\rangle = -iT H(s) |\psi(s)\rangle. \quad (3)$$

The system is initially in the ground state of  $H_i$ :  $|\psi(0)\rangle = |0; s=0\rangle$ .

At the end of the evolution we require a measure of how closely the state vector,  $|\psi(1)\rangle$ , corresponds to the desired result,  $|0; s=1\rangle$ . This is provided by the *success probability*

$$P = |\langle 0; s=1 | \psi(1) \rangle|^2. \quad (4)$$

It was shown in [1] that for  $P$  to be arbitrarily close to 1, the following condition must be satisfied:

$$T \gg \frac{\mathcal{E}}{\Delta_{\min}^2} \quad (5)$$

where

$$\mathcal{E} = \max_{0 \leq s \leq 1} \left| \left\langle 1; s \left| \frac{dH}{ds} \right| 0; s \right\rangle \right| \quad (6)$$

is of the order of a typical eigenvalue of  $H$  and

$$\Delta_{\min} = \min_{0 \leq s \leq 1} (E_1(s) - E_0(s)) \quad (7)$$

is the *minimum gap*, which occurs at reduced time(s)  $s^* : E_1(s^*) - E_0(s^*) = \Delta_{\min}$ . If  $\mathcal{E}$  is considered constant, by (5)  $\Delta_{\min}$  is the variable which determines the  $T$  that is required. It is clear that  $P$  will also be directly related to  $T$  and  $\Delta_{\min}$ . These two variables,  $P$  and  $\Delta_{\min}$ , are used interchangeably throughout the literature to quantify the performance of a given computation (e.g. contrast [2] with [3]), and are assumed to increase monotonically with each other. The question of how either of these variables varies with system size,  $n$ , is an important one that is often addressed. However, the exact nature of the relationship between these two important figures of merit has not been adequately explored.

We explore the relationship between  $P$  and  $\Delta_{\min}$  by looking at the statistical distributions of these two variables over a large set of generic problem Hamiltonians ( $H_f$ ). We start by considering a simple two-qubit system and show that a rich structure arises in the scatter plots of success probability against  $\Delta_{\min}$ . We then go on to look at the scatter plots in three-, four- and five-qubit systems and find that, although some of the finer details of the structure are washed out, some remain. We propose that the structure in the distributions arises through our choice of Hamiltonians.

## 2 A generic adiabatic algorithm

We wish to look at the distribution of the success probability and  $\Delta_{\min}$  over a large set of problem Hamiltonians. We use a simple, yet generic, model that is scalable and can be readily solved numerically. For  $H_i$ , we use a Hamiltonian that is easy to construct and whose ground state can be readily found:

$$H_i = - \sum_{i=1}^n \sigma_x^{(i)} = - \sum_{i=1}^n \mathbb{I} \otimes \cdots \otimes \sigma_x \otimes \cdots \otimes \mathbb{I}, \quad (8)$$

where  $\sigma_a$ , with  $a = x, y$  or  $z$ , denote the usual Pauli matrices,  $n$  is the number of qubits in the system and the index  $i$  denotes which qubit the operator is applied to. This  $H_i$  is simply a transverse field acting on all the qubits and its ground state is an equal superposition of all  $2^n$  computational basis states.

For  $H_f$ , we use a Hamiltonian where all possible couplings between the  $n$  qubits are realised in the  $z$ -direction, with random strengths:

$$H_f = \sum_{x=0}^{2^n-1} J_x \bigotimes_{i=1}^n (\sigma_z)^{x_i} = \sum_{y=0}^{2^n-1} f_y |y\rangle\langle y| \quad (9)$$

where  $x_i$  is the  $i$ th digit in the binary representation of  $x$  and  $J_x$  are the coupling coefficients. These will be selected from a given random distribution.  $H_f$  is diagonal in the computational basis so that the binary-ordered set of states  $|y\rangle$  is a permutation of the energy-ordered set of states  $|l; s=1\rangle$  defined in eq 2. A Hamiltonian of this type can easily be used to encode any finite computational optimisation problem (minimisation of a function  $f : \{0,1\}^n \rightarrow \mathbb{R}$ ) by choice of the  $\{J_x\}$ , including NP-hard problems such as the travelling salesman problem (TSP). It is important to note that, at present, only one- and two-qubit interactions are experimentally feasible, although the TSP can be implemented with this restriction [4].

For each sample in the scatter plots, we solve the Schrödinger equation numerically over the parameterised time,  $s$ , for a given computation time,  $T$ , using the Dormand-Prince method [5]. This is an adaptive step-size algorithm; solutions accurate to fourth- and fifth-order in  $\Delta s$  are used to estimate the local error in the former. If it is less than the desired tolerance, then the fifth-order solution is used for the integration. Otherwise the step-size  $\Delta s$  is decreased.

## 3 Two-qubit simulations

Fig. 1 is a scatter plot of success probability against minimum gap for a large set of problem instances, with the coupling coefficients drawn from the uniform distribution  $\mathcal{U}(-3,3)$ . The computation time is  $T = 5$ . Observe the sharp upper and lower edges. The lower bound of the success probability is always  $1/4$  for infinitesimally small  $\Delta_{\min}$ . This arises when  $J_1 = J_2 = J_3 = 0$ , which means there is four-fold degeneracy at  $s = 1$  and the system remains in its original ground state.

It is important to verify that this structure is independent of our choice of random distribution of coupling coefficients and that it is also not an artefact of the pseudo-random number generators used. Fig. 2 also shows scatter plots

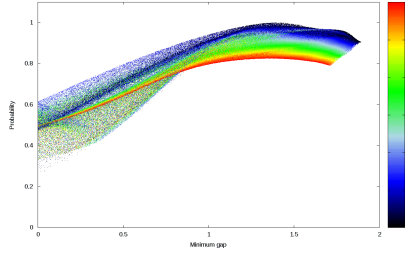


Figure 1: Success probability against minimum gap for a two-qubit system at a computation time of  $T = 5$ . The  $J_i$  have been chosen from the uniform distribution  $\mathcal{U}(-3, 3)$  for the 500,000 random problem instances. The data points are coloured by  $|J_3|$ .

of success probability and minimum gap, but in this case the coupling coefficients are drawn from a Gaussian distribution,  $\mathcal{N}(0, 1^2)$  (mean  $\mu = 0$ , standard deviation  $\sigma = 1$ ). The trends and structure in the distributions are similar to those shown in Fig. 1. However, there are some subtle differences in sharpness between the Gaussian and uniform cases. For a large minimum gap, the lowest probability occurs for large  $|J_3|$ , so we see a sharp cutoff in the uniform case and a rougher, more sparsely populated edge in the Gaussian case. In general though, this shows that the results are independent of our choice of coupling coefficients and, as a different pseudo-random number generator routine was used, we can say that the results are not a numerical artefact.

Four computation times are shown:  $T = 5, 10, 20$  and  $40$ . As this increases, the distribution shifts and tends towards a success probability of 1, as expected from the adiabatic theorem.

The two interesting features of these scatter plots are the well-defined sharp edges and the densely-populated bands. It is clear that the bands correspond to groups of Hamiltonians with similar  $|J_3|$ . The bands where  $J_3 = 0$  can be seen as two separable one-qubit evolutions for  $J_1$  and  $J_2$ , so the total success probability is simply the product of the one-qubit success probabilities. Another interesting point to note is that the bands of similar  $H_f$  gradually reverse in order in the distribution as the computation time  $T$  is changed.

We have supplemented the uniform random data with sets of  $J_i$  chosen on a rectangular grid with the same cut-offs. These have the advantage that all problem Hamiltonians with a given value of  $J_3$  can be plotted in the  $(J_1, J_2)$ -plane and coloured by their minimum gap or success probability; see Fig. 3. These two plots can be considered first- and second-order stability diagrams respectively.

The first part of Fig. 3 (minimum gap) can be explained as follows: dark

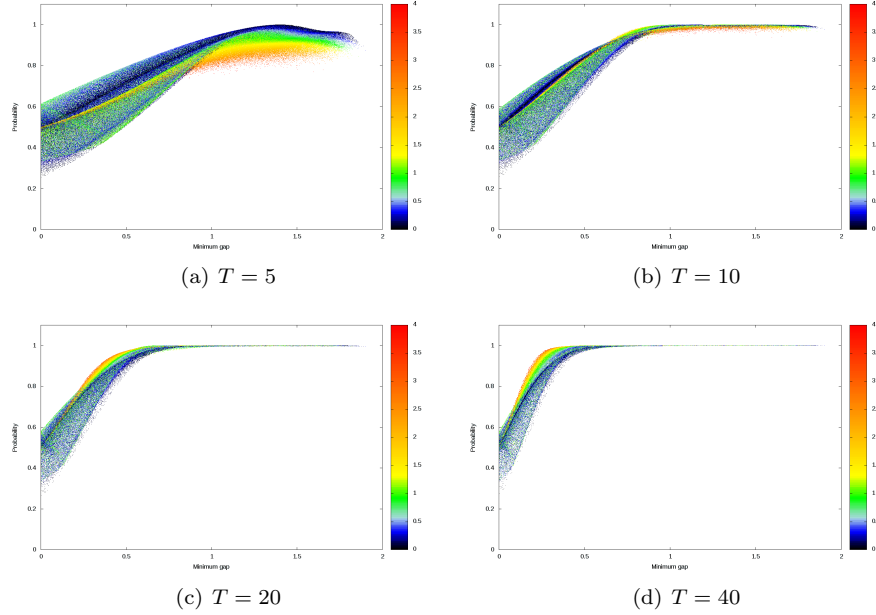


Figure 2: Success probability against minimum gap for a two-qubit system at computation times of  $T = 5, 10, 20$  and  $40$ . The  $J_i$  have been chosen from the Gaussian distribution  $\mathcal{N}(0, 1^2)$  for the 500,000 random problem instances. The data points are coloured by  $|J_3|$ .

lines correspond to problem Hamiltonians with a degenerate ground state.

$$\begin{aligned} \text{triply-degenerate} & \begin{cases} J_1 = J_2 = J_3 \\ J_1 = J_2 = -J_3 \end{cases} \\ \text{doubly-degenerate} & \begin{cases} J_1 = J_2 \text{ and } J_1, J_2 \in (-J_3, J_3) \\ J_1 = J_3 \text{ and } J_2 > J_3 \\ J_2 = J_3 \text{ and } J_1 > J_3 \\ J_1 = -J_3 \text{ and } J_2 < -J_3 \\ J_2 = -J_3 \text{ and } J_1 < -J_3 \end{cases} \end{aligned}$$

These lines separate  $H_f$  with different ground states: those in the top-right have  $|11\rangle$ ; working clockwise, the others have  $|10\rangle$ ,  $|00\rangle$  and  $|01\rangle$ .

The second part of Fig. 3 (success probability) is harder to interpret. As expected, there is a broad correspondence between lines of low  $P$  and those of low  $\Delta_{\min}$ . The difference, due to second-order corrections, is not presently understood. Nor is the interesting observation that  $H_f$  with high  $P$  are gathered around the points of triple degeneracy.

These plots suggest a projection of a surface onto the  $(\Delta_{\min}, P)$  plane; we seek to find a suitable parameterisation of the set of Hamiltonians to collapse it onto a low-dimensional surface. We find that a plot of  $P$  against the minimum gap  $\Delta_{\min}$  and the position  $s^*$  of the gap indeed shows that all points lie close to a curved surface (which rises with increasing  $T$ ). This is understandable, since

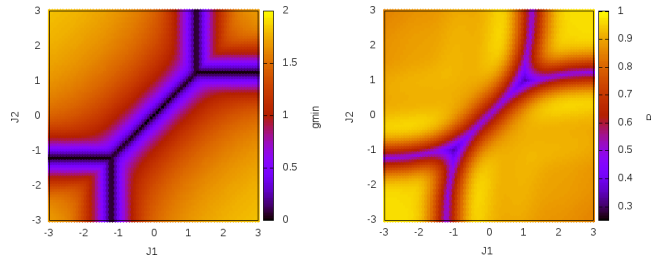


Figure 3: Minimum gap (left) and success probability (right) as a function of  $(J_1, J_2)$  at fixed  $J_3 \approx 1.22$ ,  $T = 5$ . Each coloured point in the plane is a problem Hamiltonian. Observe that points with high success probability (yellow) are nested around the points of triple degeneracy.

those two parameters largely determine the shape of the lowest two energy levels. Figure 4 shows a projection of this surface onto the  $(\Delta_{\min}, s^*)$  plane. Visual inspection shows that the colour is to a good approximation a function only of position in the plane. Note that the position of the points depends only on the Hamiltonian parameters, while the probability depends also on the computation time.

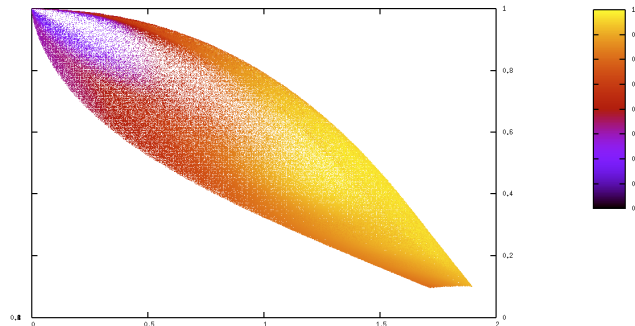


Figure 4: Scatter plot of position  $s^*$  of minimum gap against minimum gap  $\Delta_{\min}$ . The  $J_i$  have been chosen from the uniform distribution  $\mathcal{U}(-3, 3)$  for 100,000 random problem instances. Points are coloured by the success probability  $P$  at  $T = 5$ .

## 4 Larger systems

We have shown that the relationship between the success probability and  $\Delta_{\min}$  is not just a case of trivial proportionality for simple two-qubit systems. However, it is important to determine whether the interesting structure in this relationship remains in larger systems. To determine whether these densely-populated bands represent groups of problem instances that have followed similar evolution paths for the state vector (e.g. the system remaining mostly in the ground state, then being excited at a single avoided crossing), we calculated the average overlap

with the ground state:

$$\delta = \int_0^1 ds |\langle 0; s | \psi(s) \rangle|^2. \quad (10)$$

The points in Fig. 5 are coloured with respect to this average overlap value,  $\delta$ , and we can see a smooth graduation across the figures, with the average overlap with the ground state increasing with the success probability. The exception to the smooth graduation of  $\delta$  is the densely populated band where  $\delta \approx 1$ . This band must consist of cases with a degenerate or near-degenerate ground state at  $s = 1$ , as it includes cases which remain close to the instantaneous ground state throughout the majority of the evolution but have a low success probability. These results also lends credence to the idea that the structure is closely linked to the choice of Hamiltonians.

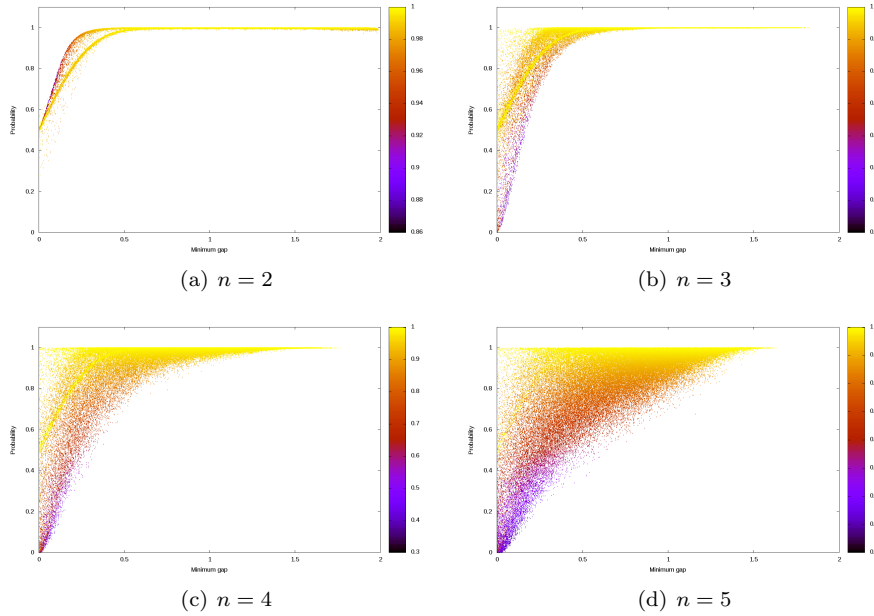


Figure 5: Distributions of success probability against  $\Delta_{\min}$  for two-, three-, four- and five-qubit systems over a set of 100,000 random problem instances, with  $T = 40$ . The colouring of the points denotes  $\delta$ , average overlap of the state vector with the instantaneous ground state.

We note that these distributions are reminiscent of the 2D projections of the higher-dimensional equilibrium surfaces seen in catastrophe theory [6]. In this case success probability,  $\Delta_{\min}$  and  $\delta$  are all internal variables of the system and not independent control parameters, so we are looking at a different situation to those usually studied in catastrophe theory. Identifying the nature of this surface and the dimensions of the phase space that it exists in is an important task, as it could have a major impact on adiabatic algorithm design. At this point we can conjecture that the constraint originates from an adiabatic invariant of the Hamiltonian. We find it strange that, to the best of our knowledge, there has been no research on adiabatic invariants of adiabatic quantum computers. A systematic investigation of adiabatic invariants of quantum computers

— especially adiabatic and approximately adiabatic computers — could yield important information about their behaviour and make a major impact on the adiabatic algorithm design.

## 5 Conclusion

We have shown that the relationship between the success probability and the minimum ground state gap may not be as straightforward as is often assumed. There is a rich structure of distinct sharp edges and densely-populated bands in the distribution, particularly in smaller systems. A partial explanation has been proposed, whereby this is the projection of a higher-dimensional surface; identification of the parameters governing this surface will guide understanding of the set of problems amenable to adiabatic quantum computing. We do not propose a definitive explanation of the origin of this rich structure: this remains an open question. However, we do suggest that there is some evidence that some of this structure could arise by our choice of Hamiltonians. We speculate that a systematic investigation of adiabatic invariants of quantum computers — especially adiabatic and approximately adiabatic computers — could yield important information about their behaviour and have a major impact on adiabatic algorithm design.

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